# Numerical Simulation of Single Droplet Dynamics with Species Diffusion for Fuel Reprocessing

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Fuel reprocessing employs liquid-liquid extraction processes to separate the components of used nuclear fuel. Two immiscible fluids (an aqueous phase and an organic phase) are counter-currently contacted, and the extraction process takes place at the liquid-liquid interface. The fluids are mixed together by mechanical action (e.g., rigorous stirring, rotation, pulsation), resulting in the dispersion of one phase into the other phase to ensure a large surface area between the phases, i.e., droplets of various size and size distribution are generated. Understanding the interface dynamics, droplet interaction, and extractant effect on droplet break-up and coalescence is very important as these small-scale phenomena can significantly affect the overall flow, and hence the extraction efficiency. Highly resolved interface dynamics simulations of the fluid flow, with species diffusion and reaction, will offer detailed information on the effects of fluid properties and flow regimes on mass transfer, drag coefficient, droplet size distribution, etc.—all required for the formulation of the reactive multiphase flow at the device scale.

To achieve this goal, we need to develop our simulation capabilities from our existing ones. As a first step, we have extended the TRUCHAS code [1] capability by coupling the current fluid-flow solver with interface tracking and surface tension [2] to the species diffusion solver [3]. The species advection term is added as a source term to the species diffusion equation. At the liquid-liquid interface, we assume thermodynamic equilibrium and assume the distribution coefficient to be unity for now.

To demonstrate the new capability, we have performed simulations in 2D and 3D of a single droplet rising by buoyancy with single species diffusion. The droplet is initially circular in 2D (spherical in 3D) in a rectangular domain, and initially contains the species. The gravitational acceleration is acting downward. We have investigated the effects of the Reynolds number on the droplet dynamics and species concentration (see Fig. 1). The Reynolds number represents the ratio between the inertial force and viscous force. As expected, we have found higher mass transfer with higher Reynolds number. We have also found our simulation results to be in agreement with the results of [4,5] for similar parameters. The droplet shape and species concentration contours for a 3D simulation are shown in Fig. 2.

Future work will include development of new capabilities to model chemical reaction, Marangoni effects, and surfactants.

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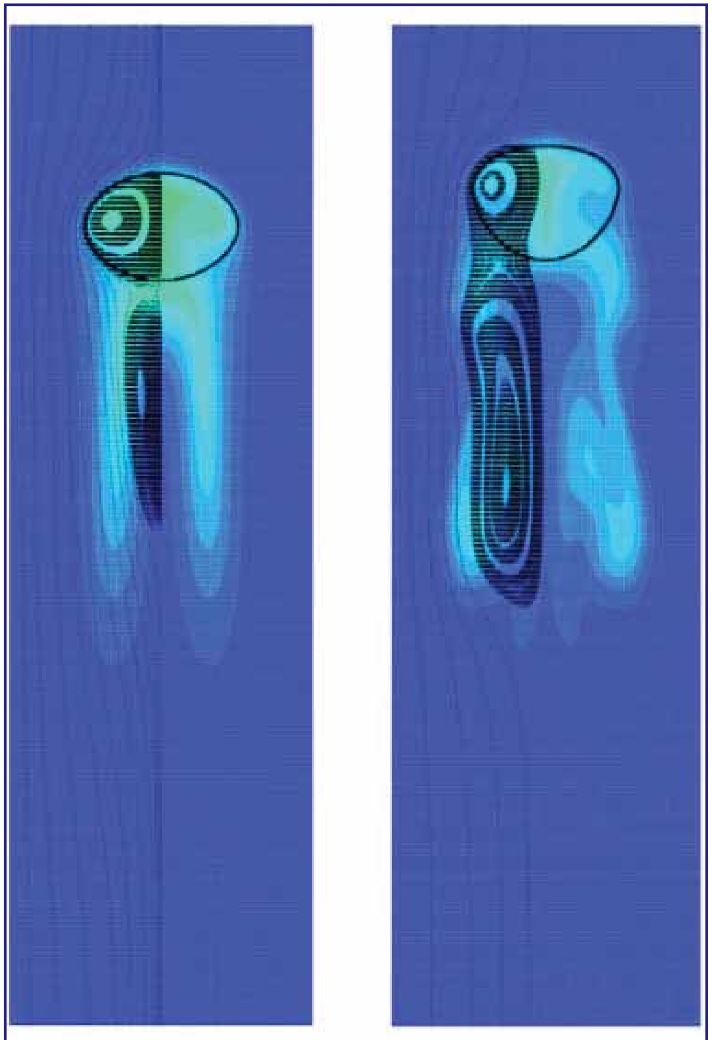


*Fig. 1. Effects of Reynolds number (Re) on 2D droplet dynamics with Weber number of 0.22 and Péclet number of 1600. The species concentration contours and droplet shape with streamtraces (on left half) are plotted at time t=1.8 in a reference frame moving with the droplet. The Weber number represents the ratio between inertia and surface tension, and the Péclet number represents the ratio between advection and diffusion.*

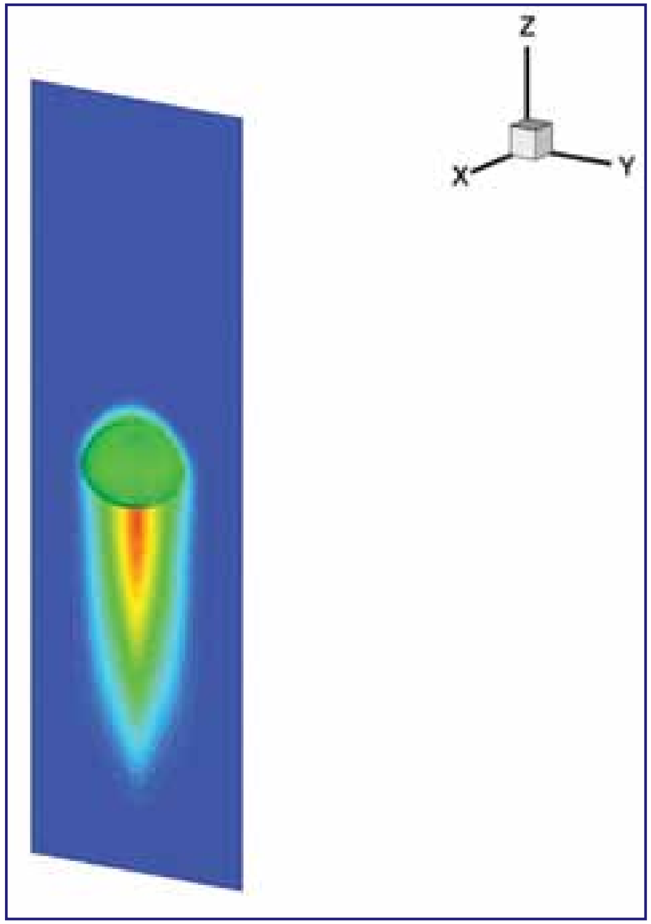


*Fig. 2. Droplet shape and species concentration contours for 3D droplet simulation at t=0.8 in mid-plane. The Reynolds number is 8, the Weber number is 0.22, and the Péclet number is 1600.*

[1] http://telluride.lanl.gov/
[2] M.M. Francois et al., *J. Comp. Phys.* **213,** 141 (2006).
[3] N.N. Carlson et al., *PEDERNAL,* LA-UR 09-07050 (2009).
[4] A. Koyonov et al., *AIChE J.* **51,** 2786 (2005).
[5] Z.-S. Mao et al., *Int. J. Heat Mass Trans.* **44,** 1235 (2001).

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